

An improvement of the Molière-Fano multiple scattering theory

A. Tarasov and O. Voskresenskaya*

Joint Institute for Nuclear Research, 141980 Dubna, Russia

Abstract

In the framework of unitary Glauber approximation for particle-atom scattering, we have received an improvement of the Molière–Fano theory (M–F theory) on the basis of reconstruction of the generalized optical theorem in it. We have estimated the relative unitary and the Coulomb corrections to the parameters of the M–F theory and studied the Z -dependence of these corrections. We showed that the absolute and relative inaccuracies of the Molière’s theory in determining the screening angle for heavy atoms of the target material ($Z \sim 80$) are about 20% and 30%, respectively.

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1 Introduction

The Molière–Fano multiple scattering theory of charged particles’ [1–3] is the most used tool for the multiple scattering effects accounting at experimental data processing. The experiment DIRAC [4, 5] like many others [6] (MuScat [7], MUCOOL [8] experiments, etc.) meets the problem of the excluding of multiple scattering effects in matter from obtained data.

The standard theory of multiple scattering [4, 6, 7], proposed by Molière [1, 2] and Fano [3], and some its modifications [7–12] are used for this aim. The modifications, developed in Refs. [7–9], are motivated by experiments

*On leave of absence from Siberian Physical Technical Institute. Electronic address: voskr@jinr.ru

[7, 8] and are connected with the inclusion to Molière theory of analogues of Fano corrections, as well as the determining their range of applicability [7–10]. In Ref. [11] is presented a modified transport equation whose solution is applicable over the range of angles, from 0 to 180°. In [12] results of experiments [13] are qualitatively explained within the framework of the theory allowing for pair correlations in the spatial distribution of scatterers.

Estimation of the theory accuracy is of especial importance in the case of DIRAC experiment for its high angular resolution. One possible source of the inaccuracy of the M–F theory is use in [1–3] an approximate expression for the amplitude of target-elastic scattering of charged particle by atom which violates the generalized optical theorem

$$\Im f_{el}(0) = \frac{k}{4\pi} \sigma_{tot} = \frac{k}{4\pi} (\sigma_{el} + \sigma_{in})$$

or, in other words, unitarity condition. Another possible source of inaccuracy is using in calculations an approximate relation for the exact and the Born values of the screening angle (χ'_a)

$$\chi'_a \approx (\chi'_a)^B \sqrt{1 + 3.34 (Z\alpha)^2}$$

obtained in the original paper Molière [1]. Therefore, the problem of estimating the M–F theory accuracy and improvement of this theory becomes important.

In the present work, we have estimated the relative unitary corrections to the parameters of the Molière–Fano theory, resulting from a reconstruction of the unitarity in the particle-atom scattering theory, and found that they are of order $Z\alpha^2$. We have also received rigorous relations between the exact and first-order parameters of the Molière multiple scattering theory, instead of the approximate one obtained in the original paper by Molière. Additionally, we evaluated absolute and relative accuracies of the Molière theory in determining the screening angle and have concluded that for heavy atoms of the target material they become significant.

The paper is organized as follows. In Section 2, we consider the approximations of the M–F theory. In Section 3, we obtain the analytical and numerical results for the unitary and the Coulomb corrections to the parameters of the M–F theory. In Conclusion, we briefly summarize our results. The some preliminary results of this work were announced in Refs. [14].

*The given work is dedicated to the
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2 Approximations of the M–F theory

2.1 Small-angle approximation

Let all scattering angles are small $\theta \ll 1$ so that $\sin \theta \sim \theta$, and the scattering problem is equivalent to diffusion in the plane of θ . Now let $\sigma_{el}(\chi)$ be the elastic differential cross section for the single scattering into the angular interval $\vec{\chi} = \vec{\theta} - \vec{\theta}'$, and $W_M(\theta, t)\theta d\theta$ is the number of scattered particles in the interval $d\theta$ after traversing a target thickness t . Then the transport equation is

$$\frac{\partial W_M(\theta, t)}{\partial t} = -n_0 W_M(\theta, t) \int \sigma_{el}(\chi) d^2\chi + n_0 \int W_M(\vec{\theta} - \vec{\chi}, t) \sigma_{el}(\chi) d^2\chi, \quad (1)$$

where $n_0 = eN_A/A$ is the number of the scattering atoms per cm^3 , N_A is the Avogadro number, and A is the atomic weight of the target atoms.

Moliere solved this equation for the determination of the spatial-angle distribution function $W_M(\theta, t)$ by the Fourier–Bessel method and gets to her a general expression

$$W_M(\theta, t) = \int_0^\infty J_0(\theta\eta) g(\eta, t) \eta d\eta, \quad (2)$$

in which

$$g(\eta, t) = \exp[N(\eta, t) - N_0(0, t)], \quad (3)$$

θ is the polar angle of the track of a scattering particle, measured with respect to the initial direction z ; η is the Fourier transform variable corresponding to θ ; and the Bessel function J_0 of order 0 is an approximate form for the Legendre polynomial appropriate to small scattering angles [2, 15].

In the notation of Molière

$$N(\eta, t) = 2\pi n_0 t \int_0^\infty \sigma_{el}(\chi) J_0(\chi\eta) \chi d\chi, \quad (4)$$

and N_0 is the value of (4) for $\eta = 0$, i.e. the total number of collisions

$$N_0(0, t) = 2\pi n_0 t \int_0^\infty \sigma_{el}(\chi) \chi d\chi. \quad (5)$$

The magnitude of $N_0 - N$ is much smaller than N_0 for values η , which are important, and may be called the ‘effective number of collisions’.

Inserting Eqs. (3)-(5) back into (2), we have

$$W_M(\theta, t) = \int_0^\infty \eta d\eta J_0(\theta\eta) \exp \left[-2\pi n_0 t \int_0^\infty \sigma_{el}(\chi) \chi d\chi [1 - J_0(\chi\eta)] \right]. \quad (6)$$

This equation is exact for any scattering law, provided only the angles are small compared with a radian.

At $g(\eta, 0) = 1$ for all η the expressions (2)-(5) can be rewritten as follows:

$$W_M(\theta, t) = \int_0^\infty J_0(\theta\eta) e^{-n_0 t Q_{el}(\eta)} \eta d\eta, \quad (7)$$

where

$$Q_{el}(\eta) = 2\pi \int_0^\infty \sigma_{el}(\chi) [1 - J_0(\chi\eta)] \chi d\chi. \quad (8)$$

This result is mathematically identical with result of Snyder and Scott for the distribution of projected angles [16].

2.2 Approximate solution of the transport equation

One of the most important results of the Molière’s theory is that the scattering is described by a single parameter, the so-called ‘screening angle’ (χ_a or χ'_a):

$$\chi'_a = \sqrt{1.167} \chi_a = [\exp(C_E - 0.5)] \chi_a \approx 1.080 \chi_a, \quad (9)$$

where $C_E = 0.57721$ is the Euler’s constant.

More precisely, the angular distribution $W_M(\theta)\theta d\theta$ depends only on the ratio of the ‘characteristic angle’ χ_c , which describes the foil thickness, to the ‘screening angle’ which describes the scattering atom:

$$b_{el} = \ln \left(\frac{\chi_c}{\chi'_a} \right)^2 \equiv \ln \left(\frac{\chi_c}{\chi_a} \right)^2 + 1 - 2C_E \sim \ln N_0. \quad (10)$$

The screening angle χ_a can be determined approximately by the relation

$$\chi_a^2 \approx \chi_0^2 (1.13 + 3.76 a^2) = (\chi_a^B)^2 (1 + 3.34 a^2) \quad (11)$$

with the so-called ‘Born parameter’

$$a = \frac{Ze^2}{\hbar v} = \frac{Z\alpha}{\beta}. \quad (12)$$

The second term in (11) represents the deviation from the Born approximation. If the value of this term is 0, the value of the screening angle is $\chi_a = \chi_a^B = \chi_0 \sqrt{1.13}$.

The angle χ_0 is defined by

$$\chi_0 = 1.13 \frac{Z^{1/3} m_e}{137 p} = \frac{Z^{1/3} m_e \alpha}{0.885 p}, \quad (13)$$

where $p = m_e v$ is momentum of incident particle and v is its velocity in the laboratory frame.

The characteristic angle is defined as

$$\chi_c^2 = 4\pi n_0 t \left(\frac{Z\alpha}{\beta p} \right)^2. \quad (14)$$

Its physical meaning is that the total probability of single scattering through an angle greater than χ_c is exactly one.

Putting $\chi_c \eta = y$ and setting $\theta/\chi_c = u$, for the most important values of η of order $1/\chi_c$, we get Molière’s transformed equation

$$W_M(\theta) \theta d\theta = u du \int_0^\infty y dy J_0(uy) \exp \left\{ -\frac{y^2}{4} \left[b_{el} - \ln \left(\frac{y^2}{4} \right) \right] \right\}, \quad (15)$$

which is very much simpler in form than (6).

In order to obtain a result valid for large all angles, Molière defines the new parameter B by the transcendental equation

$$B - \ln B = b_{el}. \quad (16)$$

The angular distribution function can be written then as

$$W_M(\theta, B) = \frac{1}{\theta^2} \int_0^\infty y dy J_0(\theta y) e^{-y^2/4} \exp \left[\frac{y^2}{4B} \ln \left(\frac{y^2}{4} \right) \right]. \quad (17)$$

The presented expansion method is to consider the term $[y^2 \ln(y^2/4)]/4B$ as a small parameter. Then the W_M is expanded in a power series in $1/B$:

$$W_M(\theta, t) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{1}{B^n} W_n(\theta, t) \quad (18)$$

with

$$W_n(\theta, t) = \frac{1}{\bar{\theta}^2} \int_0^\infty y dy J_0\left(\frac{\theta}{\bar{\theta}} y\right) e^{-y^2/4} \left[\frac{y^2}{4} \ln\left(\frac{y^2}{4}\right)\right]^n, \quad (19)$$

$$\bar{\theta}^2 = \chi_c^2 B = 4\pi n_0 t \left(\frac{Z\alpha}{pv}\right)^2 B(t).$$

This method is valid for $B \geq 4.5$ and $\bar{\theta}^2 < 1$.

The first function $W_0(\theta, t)$ have simple analytical form:

$$W_0(\theta, t) = \frac{2}{\bar{\theta}^2} \exp\left(-\frac{\theta^2}{\bar{\theta}^2}\right), \quad (20)$$

$$\bar{\theta}^2 \underset{t \rightarrow \infty}{\sim} t \ln t. \quad (21)$$

For small angles, i.e. $\theta/\bar{\theta} = \theta/(\chi_c \sqrt{B}) = \Theta$ less than about 2, the Gaussian (20) is the dominant term. In this region, $W_1(\theta, t)$ is in general less than $W_0(\theta, t)$, so that the corrections to the Gaussian is of order of $1/B$, i.e. of order of 10%.

2.3 Born approximation

On the one hand, Molière writes the elastic Born cross section for the fast charged particle scattering in the atomic field as follows:

$$\sigma_{el}^B(\chi) = \sigma^R(\chi) \left(1 - \frac{F_A(p\chi)}{Z}\right)^2 = \sigma_{el}^R(\chi) q_{el}^B(\chi). \quad (22)$$

For angles χ small compared with a radian the exact Rutherford formula has a simple approximation:

$$\sigma_{el}^B(\chi) = \frac{\chi_c^2}{4\pi n_0 t (1 - \cos \chi)^2 \chi^4} q_{el}^B(\chi) \quad (23)$$

$$\approx \frac{\theta_c^2}{\pi n_0 t \chi^4} q_{el}^B(\chi). \quad (24)$$

Here, F_A is the atomic form factor and $q_{el}^B(\chi)$ is the ratio of actual to the Rutherford scattering cross sections in the Born approximation.

Then the screening angle χ_a^B in the Born approximation one can represent via F_A or $q_{el}^B(\chi)$ by the equations

$$-\ln(\chi_a^B) = \lim_{\varsigma \rightarrow \infty} \left[\int_0^{\varsigma} \left(1 - \frac{F_A(p\chi)}{Z} \right)^2 \frac{d\chi}{\chi} + \frac{1}{2} - \ln \varsigma \right] \quad (25)$$

$$= \lim_{\varsigma \rightarrow \infty} \left[\int_0^{\varsigma} \frac{q_{el}^B(\chi) d\chi}{\chi} + \frac{1}{2} - \ln \varsigma \right] \quad (26)$$

with an angle ς such as

$$\chi_0 \ll \varsigma \ll 1/\eta \sim \chi_c \quad (27)$$

and the angle $\chi_0 \sim m_e \alpha Z^{1/3}/p$.

Molière approximation for the Thomas—Fermi form factor $F_{T-F}(q)$ with momentum transfer q can be written as

$$F_{T-F}(q)^M = \sum_{i=1}^3 \frac{c_i \lambda_i^2}{q^2 + \lambda_i^2}, \quad (28)$$

in which

$$\begin{aligned} c_1 &= 0.35, & c_2 &= 0.55, & c_3 &= 0.10, \\ \lambda_1 &= 0.30\lambda, & \lambda_2 &= 4\lambda_1, & \lambda_3 &= 5\lambda_2. \end{aligned}$$

In the case where the Born parameter $a = 0$, the equation (25) for the screening angle can be evaluated directly, using the facts that $q(0) = 0$ and $\lim_{\varsigma \rightarrow \infty} q(\varsigma) = 1$. Then with use of (22) and (28) can also be obtained the following approximation for $(\chi_a')^B$ [1, 16]:

$$(\chi_a')^B = [\exp(C_E - 0.5)] \frac{\lambda}{p} A = \sqrt{1.174} \chi_0 A, \quad (29)$$

where $\lambda = m_e \alpha Z^{1/3}/0.885$. We should note that in Refs. [1, 16] admitted a misprint, namely, the factor $A = 1.0825$ in Eq. (29) should be replaced by $A = 1.065 = \sqrt{1.13}$.

On the other hand, Molière writes the nonrelativistic Born cross section in the form

$$\sigma_{el}^B(\chi) = k^2 \left| \int_0^\infty \rho d\rho J_0 \left(2k\rho \sin \frac{\chi}{2} \right) \Phi_M^B(\vec{\rho}) \right|^2 \quad (30)$$

where the Born phase shift is given in units of $\hbar = c = 1$ by

$$\Phi_M^B(\vec{\rho}) = -\frac{2}{v} \int_{\rho}^{\infty} \frac{U_{\lambda}(r) dr}{\sqrt{r^2 - \rho^2}} = -\frac{1}{v} \int_{-\infty}^{\infty} U_{\lambda}(r = \sqrt{\rho^2 + z^2}) dz. \quad (31)$$

Here, k is the wave number of the incident particle, the variable ρ corresponds to the impact parameter of the collision, and $U_{\lambda}(r)$ is the screened Coulomb potential of the target atom

$$U_{\lambda}(r) = \pm Z \frac{\alpha}{r} \Lambda(\lambda r) \quad (32)$$

with a screening function $\Lambda(\lambda r)$. The screening radius $\lambda^{-1} = r_{sc}$ is frequently taken to be the Thomas—Fermi (T-F) radius $r_{sc} = 0.885/m_e \alpha Z^{1/3}$.

Snyder and Scott [16] have used the simplest form of (32) with a pure exponential factor $\Lambda(\lambda r) = \exp(\lambda r)$:

$$U_{\lambda}(r) = \pm Z \frac{\alpha}{r} e^{\lambda r}. \quad (33)$$

Molière in his detailed study of single scattering [1] approximated the T-F screening function by a sum of three exponentials:

$$\Lambda(\lambda r) \simeq 0.1e^{-6\lambda r} + 0.55e^{-1.2\lambda r} + 0.35e^{-0.3\lambda r}. \quad (34)$$

For the Born target-elastic single cross section have a place the following relations:

$$\frac{d\sigma_{el}^B}{d\Omega} = |f_{el}(\theta)|^2, \quad (35)$$

$$\Im f_{el}(0) = \frac{k}{4\pi} \sigma_{el}^B \neq \frac{k}{4\pi} \sigma_{tot}^B. \quad (36)$$

The Born approximation result for the amplitude f_{el} of elastic scattering of charged particle by atom reads

$$f_{el}(\theta) = ik \int_0^{\infty} J_0(\rho q) [1 - e^{i\Phi_M(\vec{\rho})}] \rho d\rho, \quad (37)$$

$$q = k\theta.$$

2.4 Approximate relation for the quantities χ_a and χ_a^B

In order to obtain a result valid for large a (i.e. not restricted to the Born approximation), Molière uses in his calculations of the screening angle a WKB technique.

The exact formulas for the WKB differential cross section $\sigma_{el}(\chi)$ and corresponding $q_{el}(\chi)$ in terms of an integral are given in Molière's paper [1] as follows:

$$\sigma_{el}(\chi) = k^2 \left| \int_0^\infty \rho d\rho J_0(k\chi\rho) \left\{ 1 - \exp [i\Phi_M(\vec{\rho})] \right\} \right|^2, \quad (38)$$

$$q_{el}(\chi) = \frac{(k\chi)^4}{4a^2} \left| \int_0^\infty \rho d\rho J_0(k\chi\rho) \left\{ 1 - \exp [i\Phi_M(\vec{\rho})] \right\} \right|^2 \quad (39)$$

with the phase shift given by

$$\Phi_M(\vec{\rho}) = \int_{-\infty}^\infty [k_r(r) - k] dz, \quad (40)$$

where $k_r(r)$ is the relativistic wavenumber for the particle at a distance r from the nucleus, and the quantity ρ is seen to be impact parameter of the trajectory or 'ray'. As before, k is the initial or asymptotic value of the wavenumber.

When $k_r(r)$ is expanded as a series of powers of $U_\lambda(r)/k$, then the first-degree term yields the same expression for $\Phi_M(\vec{\rho})$ as Eq. (31). The Born approximation for (38) is obtained by expanding the exponential in (38) to first order in parameter a (12).

Relations (24) and (52) between the quantities $\sigma_{el}^B(\chi)$, $q_{el}^B(\chi)$, and χ_a^B remain valid also for $\sigma_{el}(\chi)$, $q_{el}(\chi)$, and χ_a .

Despite the fact that the formulas (38), (39) are exact, evaluation of these quantities was carried out by Molière only approximately.

To estimate (39), Molière used the first-order Born shift (31) with (32) and (34), what is good only to terms of first order in a , and found

$$q_{el}(\chi) \approx \left| 1 - \frac{4ia(1-ia)^2}{(\chi/\chi_0)^2} \left\{ -0.81 + 2.21 \left[-\Re[\psi(ia)] - \frac{1}{1-ia} + \frac{1}{2ia} + \lg \frac{\chi}{2\chi_0} \right] \right\} \right|^2. \quad (41)$$

Here, ψ is the so-called ‘digamma function’, i.e. the logarithmic derivative of the Γ -function $\psi(x) = d \ln \Gamma(x)/dx$.

He has fitted a simple formula to the function $\Re[\psi(ia)]$ in Eq. (41)

$$\Re[\psi(ia)] \approx \frac{1}{4} \lg \left(a^4 + \frac{a^2}{3} + 0.13 \right). \quad (42)$$

Using (42) in Eq. (41) and expanding with neglect of higher orders in a^2 and $(\chi/\chi_0)^{-2}$, he got

$$q_{el}(\chi) \approx 1 - \frac{8.85}{(\chi/\chi_0)^2} \left[1 + 2.303 a^2 \lg \frac{7.2 \cdot 10^{-4} (\chi/\chi_0)^4}{(a^4 + a^2/3 + 0.13)} \right]. \quad (43)$$

Molière has calculated $q_{el}(\chi)$ for different values of a and as a result has devised an interpolation scheme, based on a linear relation between $(\chi/\chi_0)^2$ and a^2 for fixed q_{el} :

$$(\chi/\chi_0)^2 \approx A_q + a^2 B_q. \quad (44)$$

Calculating the screening angle defined by

$$-\ln(\chi_a) = \frac{1}{2} + \lim_{\varsigma \rightarrow \infty} \left[\int_0^\varsigma \frac{q_{el}(\chi) d\chi}{\chi} - \ln \varsigma \right] = \frac{1}{2} - \ln \chi_0 - \int_0^1 dq \ln \left(\frac{\chi}{\chi_0} \right) \quad (45)$$

and assuming a linear relation between χ_a^2 and a^2 , Molière writes finally the following interpolating formula:

$$\chi_a \approx \chi_0 \sqrt{1.13 + 3.76 a^2}. \quad (46)$$

Critical remarks to his conclusion see in the review of V.T. Scott [16].

2.5 Fano approximation

To estimate a contribution of incoherent scattering on atomic electrons is often [2, 3, 15, 17] replaced the squared nuclear charge Z^2 with the sum of the squares of the nuclear and electronic charges $Z(Z+1)$ in basic relations (for differential cross-section, some parameters of the theory, etc.).

This procedure would be accurate if the single-scattering cross sections were the same for nucleus and electron targets. Besides, the actual cross sections are different at small and large angles. Fano modified the multiple scattering theory taking into account above differences.

For this purpose Fano separates the elastic and inelastic contributions to the cross sections

$$\sigma(\chi) = \sigma_{el}(\chi) + \sigma_{in}(\chi). \quad (47)$$

For the inelastic components of the single scattering differential cross sections, the Fano approximation reads

$$\frac{d\sigma_{in}}{d\Omega} = \frac{d\sigma_{in}^B}{d\Omega}. \quad (48)$$

Since the Born single-scattering amplitudes are pure real, the generalized optical theorem cannot be used to calculate the total cross section in the framework of this approximation.

Fano sets the task of comparing the contribution of $\sigma_{in}^B(\chi)$ to the exponent of the Goudsmit—Saunderson distribution¹ [18] for total scattering angle:

$$W(\theta, t) = 2\pi \sum_l \left(l + \frac{1}{2} \right) P_l(\theta) \exp \left\{ -n_0 t \int \sigma^B(\chi) \sin \chi d\chi [1 - P_l(\chi)] \right\}, \quad (49)$$

where P_l is the Legendre polynomial. If we replace in (49) the sum over l by an integral over η , $(l + \frac{1}{2})$ by η , P_l by the well-known formula $P_l(\theta) = J_0((l + \frac{1}{2})\theta)$, and $\sin \chi$ by χ , the expression (49) goes over into small-angle distribution (6) of Molière and Lewis.

To achieve the mentioned goal in the small-angle approximation, we determine in accordance with [15] and [9] similarly to (23) and (25) the corresponding expressions for the inelastic cross section

$$\sigma_{in}^B(\chi) = \sigma^R(\chi) q_{in}^B(\chi) = \frac{\chi_c^2}{4\pi n_0 t Z (1 - \cos \chi)^2 \chi^4} q_{in}^B(\chi) \quad (50)$$

$$\approx \frac{\chi_c^2}{\pi n_0 t Z \chi^4} q_{in}^B(\chi) \quad (51)$$

and the ‘inelastic cut-off angle’ χ_{in}^B

$$-\ln(\chi_{in}^B) = \lim_{\zeta \rightarrow \infty} \left[\int_0^\zeta \frac{q_{in}^B(\chi) d\chi}{\chi} + \frac{1}{2} - \ln \zeta \right]. \quad (52)$$

¹ The Goudsmit—Saunderson theory is valid for any angle, small or large, and do not assume any special form for the differential scattering cross section.

Then, with the use of (23) and (51), angular distribution (17) can be rewritten as follows

$$W_{M-F}(\Theta, B) = \frac{1}{\theta^2} \int_0^\infty y dy J_0(\Theta y) e^{-y^2/4} \exp(Y_{el} + Y_{in}) \quad (53)$$

with

$$Y_{el} = \frac{y^2}{4B} \ln\left(\frac{y^2}{4}\right), \quad Y_{in} = \frac{2y^2}{(Z+1)B} \int_\zeta^\infty [1 - J_0(\Theta)] \Theta^{-3} d\Theta, \quad (54)$$

where the parameter B is defined by equation

$$B - \ln B = b_{el} + b_{in}, \quad (55)$$

in which

$$b_{el} = \ln\left(\frac{\chi_c}{\chi_a^B}\right)^2 + 1 - 2C_E, \quad b_{in} = \frac{1}{Z+1} \ln\left(\frac{\chi_a^B}{\chi_{in}^B}\right)^2. \quad (56)$$

Numerical estimation of the $-u_{in} = -\ln(\chi_{in}^B)^2$ value from the T-F model yields $(-u_{in})_{T-F} = 5.8$ for all Z . The value of $-u_{in}$ should not vary greatly from one material to another.

For sufficiently large angles, with the use of exact Rutherford formulas (23) and (50), the correct angular distribution $W(\theta, t)$ may be estimated according to the formula

$$W_{corr}(\theta, t) = W(\theta, t) [\sigma_{exact}^B(\chi)/\sigma^R(\chi)], \quad (57)$$

as suggested Bethe [15] and Fano [3].

3 Improvement of the M-F theory

3.1 Glauber approximation

The Glauber approximation [19] for the amplitude $F_{if}(\vec{q})$ of the multiple scattering at small angles is given by

$$F_{if}(\vec{q}) = \frac{ik}{2\pi} \int d^2\rho \exp(i\vec{q}\vec{b}) \Gamma_{if}(\vec{\rho}), \quad (58)$$

where $\Gamma_{if}(\vec{\rho})$ is so-called ‘profile function’.

We may formulate the problem in a general way by considering the scattering of a pointlike projectile on a system of Z constituents with the coordinates $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_Z$ and the projections on the plane of the impact parameter $\vec{s}_1, \vec{s}_2, \dots, \vec{s}_Z$. Then we may write the total phase shift as a sum of the form

$$\tilde{\chi}(\vec{\rho}, \vec{x}_1, \vec{x}_2, \dots, \vec{x}_Z) = \sum_{k=1}^Z \tilde{\chi}_k(\vec{\rho} - \vec{s}_k). \quad (59)$$

If we introduce the configuration space of the wave functions ψ_i and ψ_f for the initial and final constituents states, we may write the profile function as

$$\Gamma_{if}(\vec{\rho}) = \int \prod_{k=1}^Z d^3r_k \psi_f^*(\{\vec{r}_k\}) \psi_i(\{\vec{r}_k\}) \Gamma(\vec{\rho}, \{\vec{s}_k\}) \quad (60)$$

with the interaction operator

$$\Gamma(\vec{\rho}, \{\vec{s}_k\}) = 1 - \exp[i\Phi(\vec{\rho}, \{\vec{s}_k\})] \quad (61)$$

and the phase-shift function

$$\tilde{\Phi}(\vec{\rho}, \{\vec{s}_k\}) = Z\tilde{\chi}(\vec{\rho}) - \sum_{k=1}^Z \tilde{\chi}(\vec{\rho} - \vec{s}_k). \quad (62)$$

When the interaction is due to a potential $V(\vec{r})$, the phase function $\tilde{\chi}(\vec{\rho})$ is given by

$$\tilde{\chi}(\vec{\rho}) = -\frac{1}{v} \int_{-\infty}^{\infty} V\left(\sqrt{\rho^2 + z^2}\right) dz. \quad (63)$$

with the potential of an individual constituent's

$$V(r) = \pm \lim_{\lambda \rightarrow 0} \frac{\alpha}{r} e^{-\lambda r}, \quad \lambda \sim m_e \alpha Z^{1/3}. \quad (64)$$

The multiple-scattering amplitude $F_{if}(\vec{q})$ (58) is normalized by the relations:

$$4\pi \Im F_{ii}(0) = \sigma(i)_{tot}, \quad |F_{if}(\vec{q})|^2 = d\sigma_{if}/dq_T, \quad (65)$$

where

$$\sigma(i)_{tot} = \sigma(i)_{el} + \sigma(i)_{in}, \quad \sigma_{if} = \int |d\sigma_{if}/dq_T|^2 d^2q, \quad (66)$$

$$\sigma(i)_{tot} = \sum_f \sigma_{if}. \quad (67)$$

In terms of $e^{i\tilde{\Phi}}$, where the phase-shift function $\tilde{\Phi} = \tilde{\Phi}(\vec{\rho}, \{\vec{s}_k\})$ is given by (62), the cross sections $\sigma(i)_{tot}$, $\sigma(i)_{el}$, $\sigma(i)_{in}$ could be written as follows:

$$\sigma(i)_{tot} = 2\Re \int \left\langle 1 - \left\langle e^{i\tilde{\Phi}} \right\rangle \right\rangle d^2\rho, \quad (68)$$

$$\sigma(i)_{el} = \int \left\langle 1 - 2\Re \left\langle e^{i\tilde{\Phi}} \right\rangle + \left| \left\langle e^{i\tilde{\Phi}} \right\rangle \right|^2 \right\rangle d^2\rho, \quad (69)$$

$$\sigma(i)_{in} = \int \left\langle 1 - \left| \left\langle e^{i\tilde{\Phi}} \right\rangle \right|^2 \right\rangle d^2\rho. \quad (70)$$

The brackets $\left\langle e^{i\tilde{\Phi}} \right\rangle$ signify that an overage is be taken over all configurations of the target constituents in i -th state.

3.2 Reconstruction of unitary conditions

To reduce the many-body problem to the consideration of an effective one-body problem and to establish the relationship between the Glauber and the Molière theories, we introduce the abbreviation

$$\left\langle e^{i\tilde{\Phi}} \right\rangle = e^{i\bar{\Phi}} \quad (71)$$

and consider for the effective ('optical') phase shift function $\bar{\Phi}(\vec{\rho})$ the expansion

$$\bar{\Phi}(\vec{\rho}) = \sum_{n=1}^{\infty} \frac{i^{n-1}}{n!} \Phi_n, \quad (72)$$

where

$$\begin{aligned} \Phi_1 &= \langle \Phi \rangle, \quad \Phi_2 = \langle (\Phi - \Phi_1)^2 \rangle, \\ \Phi_3 &= \langle (\Phi - \Phi_1)^3 \rangle, \dots, \Phi_n \sim Z\alpha^n/\beta. \end{aligned} \quad (73)$$

The first order of the expression for $\bar{\Phi}(\vec{\rho})$ is simply the average of the function $\tilde{\Phi}(\vec{\rho}, \{\vec{s}_k\})$ and correspond to the first-order Born approximation. The second order term of $\bar{\Phi}(\vec{\rho})$ is purely absorptive (i.e., positive imaginary) in character and is equal in order of magnitude to the $Z\alpha^2/\beta$.

When in the expansion (72)

$$\overline{\Phi}_{tail}(\vec{\rho}) = \sum_{n=3}^{\infty} \frac{i^{n-1}}{n!} \Phi_n \ll 1, \quad (74)$$

it seems natural to neglect the $\overline{\Phi}_{tail}(\vec{\rho})$ and consider the following approximation:

$$\overline{\Phi}(\vec{\rho}) \approx \Phi_1(\vec{\rho}) + \frac{i}{2} \Phi_2(\vec{\rho}), \quad (75)$$

in which we let $\Phi_1(\vec{\rho}) = \Phi_M(\vec{\rho})$ and $\Phi_2(\vec{\rho}) = 2\Phi_{in}(\vec{\rho})$. The last term correspond to target-inelastic scattering, also referred to as incoherent scattering or ‘antiscreeing’ [5].

This leads to the following improvement of the Molière–Fano theory:

$$\Phi_M(\vec{\rho}) \Rightarrow \Phi_M(\vec{\rho}) + i\Phi_{in}(\vec{\rho}) \quad (76)$$

with

$$2\Phi_{in}(\vec{\rho}) = \lim_{\lambda \rightarrow 0} Z \left\{ \int |\tilde{\chi}_\lambda(\vec{\rho} - \vec{r}_T)|^2 \varrho(\vec{r}) d^3r - \left| \int \tilde{\chi}_\lambda(\vec{\rho} - \vec{r}_T) \varrho(\vec{r}) d^3r \right|^2 \right\}, \quad (77)$$

where

$$\tilde{\chi}_\lambda(\vec{\rho}) = -\frac{1}{v} \int_{-\infty}^{\infty} V_\lambda \left(\sqrt{\rho^2 + z^2} \right) dz, \quad V_\lambda(r) = \mp \frac{\alpha}{r} e^{-\lambda r}, \quad (78)$$

$$\varrho(\vec{r}) = \psi_f^*(\vec{r}) \psi_i(\vec{r}). \quad (79)$$

For the cross sections

$$\sigma_{tot} = \langle \sigma(i)_{tot} \rangle, \quad \sigma_{in} = \langle \sigma(i)_{in} \rangle, \quad \sigma_{el} = \langle \sigma(i)_{el} \rangle, \quad (80)$$

takes place the unitary condition

$$\Im f_{el}(0) = \frac{k}{4\pi} \sigma_{tot} = \frac{k}{4\pi} (\sigma_{el} + \sigma_{in}) \quad (81)$$

with

$$f_{el}(\theta) = F_{ii}(\vec{q}), \quad \Im F_{ii}(0) = \frac{k}{4\pi} \sum_f \int |F_{if}(\vec{q})|^2 d\Omega, \quad (82)$$

$$\frac{d\sigma_{in}}{d\Omega} = \sum_{f \neq i} |F_{if}(\vec{q})|^2, \quad F_{if}(\vec{q}) = \frac{ik}{2\pi} \int d^2\rho \exp(i\vec{q}\vec{\rho}) \Gamma_{if}(\vec{\rho}), \quad (83)$$

$$\Gamma_{if}(\vec{\rho}) = 1 - \exp(-2\Phi_{in}), \quad (84)$$

$$q = k\theta.$$

Using (81), we found for the cross sections the following expressions:

$$\sigma_{tot} = 4\pi \int (1 - \cos \Phi_M(\vec{\rho}) e^{-\Phi_{in}(\vec{\rho})}) \rho d\rho, \quad (85)$$

$$\sigma_{in} = 2\pi \int (1 - e^{-2\Phi_{in}(\vec{\rho})}) \rho d\rho, \quad (86)$$

$$\sigma_{el} = 2\pi \int (1 - 2\cos \Phi_M(\vec{\rho}) e^{-\Phi_{in}(\vec{\rho})} + e^{-2\Phi_{in}(\vec{\rho})}) \rho d\rho. \quad (87)$$

3.3 Unitary corrections to the Born approximation

With the use of the evaluation formula

$$\int [2\Phi_{in}(\vec{\rho})] d^2\rho \sim Z\alpha^2/\beta \quad (88)$$

and the exact contributions have been calculated in [20], we obtain the following unitary relative correction δ_{unit} to the first-order Born cross section of the inelastic scattering σ_{in}^B :

$$\delta_{unit} = \frac{\Delta \sigma_{in}}{\sigma_{in}^B} = \frac{\sigma_{in} - \sigma_{in}^B}{\sigma_{in}^B} = \frac{\sigma_{in}}{\sigma_{in}^B} - 1 \sim Z\alpha^2/\beta \quad (89)$$

with

$$\sigma_{in}^B = \left\langle \int \Phi_{in}(\vec{\rho}) d^2\rho \right\rangle. \quad (90)$$

The corresponding angular distribution reads

$$W_{in}(\theta) = 2\pi \int_0^\infty J_0(\theta\eta) e^{-Q_{in}(\eta)} \eta d\eta, \quad (91)$$

$$Q_{in}(\eta) = 2\pi \int \sigma_{in}(\theta)[1 - J_0(\theta\eta)]\theta d\theta. \quad (92)$$

Inserting Eq. (92) back into (91), we get the equation of the form:

$$W_{in}(\theta) = 2\pi \int_0^\infty \eta d\eta J_0(\theta\eta) \exp \left[-2\pi \int_0^\infty \sigma_{in}(\theta')\theta' d\theta' [1 - J_0(\theta'\eta)] \right]. \quad (93)$$

With the use of

$$\int \eta J_0(\theta\eta) J_0(\theta'\eta) d\eta = \frac{1}{\theta} \delta(\theta - \theta') = 0 \quad (94)$$

and

$$\int_0^\infty d\eta \eta J_0(\theta\eta) = 2a^{-2} \frac{\Gamma(1)}{\Gamma(0)} = 0, \quad \int_0^\infty d\eta \eta J_0(\theta\eta) J_0(\theta'\eta) = 0, \quad (95)$$

according to [21], the integration of Eq. (93) yields the following result:

$$W_{in}(\theta) = -(2\pi)^2 \int_0^\infty \eta J_0(\theta\eta) J_0(\theta'\eta) d\eta \cdot \sigma_{in}(\theta')\theta' d\theta' = -(2\pi)^2 \sigma_{in}(\theta). \quad (96)$$

In Eqs. (94) and (95) δ is the Dirac delta function and Γ is the Euler Gamma function.

Finally, taking into account the relations (89) and (96), we can estimate the unitary correction to the angular distribution function (91):

$$\delta_{unit} = \frac{\Delta W_{in}(\theta)}{W_{in}^B(\theta)} = \frac{W_{in}(\theta)}{W_{in}^B(\theta)} - 1 = \frac{\sigma_{in}(\theta)}{\sigma_{in}^B(\theta)} - 1 = \frac{\sigma_{in}}{\sigma_{in}^B} - 1 \sim Z\alpha^2/\beta. \quad (97)$$

3.4 Rigorous relations between exact and Born results

To obtain an exact correction to the Born screening angle $(\chi'_a)^B$ in small-angle approximation, we will carry out our analytical calculation in terms of the function $Q_{el}(\eta)$ (8):

$$Q_{el}(\eta) = 2\pi \int_0^\infty \sigma_{el}(\chi)[1 - J_0(\chi\eta)]\chi d\chi \equiv \int d^2\rho [1 - \cos[\Delta\Phi(\vec{\rho}, \vec{\eta})]], \quad (98)$$

where the phase shift is determined by the equation

$$\Delta\Phi(\vec{\rho}, \vec{\eta}) = \Phi(\rho_+) - \Phi(\rho_-), \quad \vec{\rho}_{\pm} = \vec{\rho} \pm \vec{\eta}/2p. \quad (99)$$

Substituting the expression for the cross section

$$\sigma_{el}(\chi) = \frac{\chi_c^2}{\pi n_0 t \chi^4} q_{el}(\chi) \quad (100)$$

into (98), we rewrite it in the form:

$$n_0 t Q_{el}(\eta) = 2\chi_c^2 \int_0^\infty [1 - J_0(\chi\eta)] q_{el}(\chi) \chi^{-3} d\chi. \quad (101)$$

For the important values of η of order $1/\chi_c$ or less, it is possible to split the last integral at the angle ς (27) into two integrals:

$$\begin{aligned} I(\eta) &= \int_0^\infty [1 - J_0(\chi\eta)] q_{el}(\chi) \chi^{-3} d\chi \\ &= \int_0^\varsigma [1 - J_0(\chi\eta)] q_{el}(\chi) \chi^{-3} d\chi + \int_\varsigma^\infty [1 - J_0(\chi\eta)] q_{el}(\chi) \chi^{-3} d\chi \\ &= I_1(\varsigma\eta) + I_2(\varsigma\eta). \end{aligned} \quad (102)$$

For the part from 0 to ς , we may write $1 - J_0(\chi\eta) = \chi^2\eta^2/4$, and the integral I_1 reduces to a universal one, independently of η :

$$I_1(\varsigma\eta) = \frac{\eta^2}{4} \int_0^\varsigma q_{el}(\chi) d\chi/\chi. \quad (103)$$

For the part from ς to infinity, the quantity $q_{el}(\chi)$ can be replaced by unity, and the integral I_2 can be integrated by parts. This leads to the following result for I_2 :

$$I_2(\varsigma\eta) = \frac{\eta^2}{4} \left[1 - \ln(\varsigma\eta) + \ln 2 - C_E + O(\varsigma\eta) \right]. \quad (104)$$

Integrating (103) with the account (45), substituting obtained solutions back into (101), and also using definition

$$\ln(\chi_c/\chi_a)^2 + 1 - 2C_E = \ln(\chi_c/\chi'_a)^2,$$

as a result for $Q_{el}(\eta)$, we obtain:

$$\begin{aligned} Q_{el}(\eta) &= -\frac{(\chi_c \eta)^2}{2n_0 t} \left[\ln \left(\frac{\chi_c^2 \eta^2}{4} \right) - \ln \left(\frac{\chi_c}{\chi'_a} \right)^2 \right] \\ &= -\frac{(\chi_c \eta)^2}{2n_0 t} \ln \left(\frac{\eta^2 (\chi'_a)^2}{4} \right). \end{aligned} \quad (105)$$

Finally, considering definition of χ_c (14), we can represent $Q_{el}(\eta)$ by the following expression:

$$Q_{el}(\eta) = -2\pi \left(\frac{Z\alpha}{\beta p} \right)^2 \eta^2 \ln \left(\frac{\eta^2 (\chi'_a)^2}{4} \right). \quad (106)$$

Then, the screening angle χ'_a can be determined via $Q_{el}(\eta)$ by a linear equation:

$$-\ln (\chi'_a)^2 = \ln \left(\frac{\eta^2}{4} \right) + \left[2\pi \eta^2 \left(\frac{Z\alpha}{\beta p} \right)^2 \right]^{-1} Q_{el}(\eta). \quad (107)$$

Let us present the quantity $Q_{el}(\eta)$ in the form:

$$Q_{el}(\eta) = Q_{el}^B(\eta) - \Delta_{CC}[Q_{el}(\eta)]. \quad (108)$$

Then, on the one hand, using (106), the difference $\Delta_{CC}[Q_{el}(\eta)]$ between the Born approximate $Q_{el}^B(\eta)$ and exact in the Born parameter values of the quantity $Q_{el}(\eta)$ can be reduced to a difference in the quantities $\ln (\chi'_a)$ and $\ln (\chi'_a)^B$:

$$\begin{aligned} \Delta_{CC}[Q_{el}(\eta)] &\equiv Q_{el}^B(\eta) - Q_{el}(\eta) \\ &= 4\pi \eta^2 \left(\frac{Z\alpha}{\beta p} \right)^2 \left[\ln (\chi'_a) - \ln (\chi'_a)^B \right] \equiv 4\pi \eta^2 \left(\frac{Z\alpha}{\beta p} \right)^2 \Delta_{CC}[\ln (\chi'_a)]. \end{aligned} \quad (109)$$

On the other hand, this difference can be reduced to a difference $\Delta q_{el}(\chi) = q_{el}^B(\chi) - q_{el}(\chi)$:

$$\Delta_{CC}[Q_{el}(\eta)] = 2\pi \int_0^\infty \chi d\chi \Delta \sigma_{el}(\chi) [1 - J_0(\chi \eta)] = \frac{2\chi_c^2}{n_0 t} \int_0^\infty \frac{d\chi}{\chi^3} \Delta q_{el}(\chi) [1 - J_0(\chi \eta)],$$

and for (39) with (99), as a result of integration, (110) becomes

$$\begin{aligned}\Delta_{CC}[Q_{el}(\eta)] &= 4\pi\eta^2 \left(\frac{Z\alpha}{\beta p}\right)^2 \left[\frac{1}{2}\psi\left(i\frac{Z\alpha}{\beta}\right) + \frac{1}{2}\psi\left(-i\frac{Z\alpha}{\beta}\right) - \psi(1) \right] \\ &= 4\pi\eta^2 \left(\frac{Z\alpha}{\beta p}\right)^2 \left\{ \Re \left[\psi\left(1 + i\frac{Z\alpha}{\beta}\right) \right] + C_E \right\},\end{aligned}\quad (110)$$

where

$$\begin{aligned}\Re[\psi(1 + ia)] &= \Re[\psi(1 - ia)] = \Re[\psi(ia)] = \Re[\psi(-ia)] \\ &= -C_E + a^2 \sum_{n=1}^{\infty} \frac{1}{n(n^2 + a^2)} = -C_E + f(a),\end{aligned}\quad (111)$$

$$-\infty < a < \infty,$$

$\psi(1) = -C_E$, and $f(a) = a^2 \sum_{n=1}^{\infty} [n(n^2 + a^2)]^{-1}$ is an ‘universal function of $a = Z\alpha/\beta$ ’.

As consequence, we can get the following rigorous relations between the quantities $\ln(\chi'_a)$ and $\ln(\chi'_a)^B$:

$$\ln(\chi'_a) - \ln(\chi'_a)^B = \Re[\psi(1 + ia) - \psi(1)], \quad (112)$$

$$\Delta_{CC}[\ln(\chi'_a)] = a^2 \sum_{n=1}^{\infty} [n(n^2 + a^2)]^{-1}. \quad (113)$$

We point out that the relations (110), (112), and (113) are independent on the form of electron distribution in atom and are valid for any atomic model.

From (110) also follows an expression for the correction to the exponent of (6). Since $\ln[g(\eta)] = -n_0 t Q$, we get:

$$\Delta_{CC}[\ln g(\eta)] \equiv \ln[g(\eta)] - \ln[g^B(\eta)] \quad (114)$$

$$= 4\pi\eta^2 n_0 t \left(\frac{Z\alpha}{\beta p}\right)^2 f(a).$$

For the specified value of $\eta^2 = 1/\chi_c^2$, using the definition of χ_c (14), we can evaluate this correction:

$$\Delta_{CC}[\ln g(\chi_c)] = \frac{4\pi n_0 t}{\chi_c^2} \left(\frac{\chi_c^2}{4\pi n_0 t}\right)^2 f(a) = f(a). \quad (115)$$

The formulas for the so-called ‘Coulomb correction’ (CC), defined as a difference between the exact and the Born approximate results, are known as the Bethe—Bloch formulas for the ionization losses [22] and the formulas for the Bethe—Heitler cross section of bremsstrahlung [23].

The similar expression was found for the total cross section of the Coulomb interaction of compact hadronic atoms with ordinary target atoms [24]. The more complicate formal expression for CC was derived by I. Øverbø in [25].

Were also obtained CC to the cross sections of the pair production in nuclear collisions [26, 27], as well as to the solutions of the Dirac and Klein-Gordon equations [28]. Specificity of the expressions received in the present work is that they define CC not to the cross sections of the processes, but to screening angle and an exponential part of the distribution function.

3.5 Relative Coulomb corrections to the Born approximation

Let us write (113) in the following way

$$(\chi'_a) = (\chi'_a)^B \exp \left[f \left(\frac{Z\alpha}{\beta} \right) \right]. \quad (116)$$

The exact (Coulomb) relative corrections to the Born screening angle $(\chi'_a)^B$ can be then represented as follows

$$\delta_{CC}(\chi'_a) = \frac{\chi'_a - (\chi'_a)^B}{(\chi'_a)^B} = \frac{\Delta(\chi'_a)}{(\chi'_a)^B} = \exp \left[f \left(\frac{Z\alpha}{\beta} \right) \right] - 1. \quad (117)$$

The relative CC to the exponent $g^B(\eta)$ at $\eta^2 = 1/\chi_c^2$, as follows from (115), is also determined by this quantity: $\delta_{CC}(\chi'_a) = \delta_{CC}[g(\chi_c)]$. Moreover, because

$$\Delta W(\chi_c, t) \equiv W_M - W_M^B = \int_0^\infty J_0(\theta\eta) \Delta g(\chi_c) \eta d\eta, \quad (118)$$

accounting $\int_0^\infty d\eta \eta J_0(\theta\eta) = 0$, we get

$$\delta_{CC}[W_M(\chi_c, t)] = \frac{\Delta W(\chi_c, t)}{W^B(\chi_c, t)_M} = \frac{\Delta g(\chi_c)}{g^B(\chi_c)} = \exp \left[f \left(\frac{Z\alpha}{\beta} \right) \right] - 1. \quad (119)$$

Thus,

$$\delta_{CC} \equiv \delta_{CC}(\chi'_a) = \delta_{CC}[g(\chi_c)] = \delta_{CC}[W_M(\chi_c, t)].$$

To compare the second-order relative corrections to the first-order results, which correspond to Eqs. (116) and (11), respectively, we first present these equations in the following approximate form:

$$(\chi'_a) \approx (\chi'_a)^B \left[1 + 1.204 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right) \right], \quad (120)$$

$$(\chi'_a) \approx (\chi'_a)^B \left[1 + 1.670 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right) \right]. \quad (121)$$

The last expression follows from

$$\chi_a \approx \chi_a^B \sqrt{1 + 3.34 \left(\frac{Z\alpha}{\beta} \right)^2} \approx \chi_a^B \left[1 + 1.670 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right) \right],$$

where $\chi_a = (\chi'_a)/1.080$ and $\chi_a^B = (\chi'_a)^B/1.080$. Then, (120) and (121) becomes

$$\delta_{CC}^{(2)}(\chi'_a) \approx \frac{\Delta(\chi'_a)}{(\chi'_a)^B} \approx 1.204 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right), \quad (122)$$

$$\delta_M^{(2)}(\chi'_a) \approx \frac{\Delta(\chi'_a)}{(\chi'_a)^B} \approx 1.670 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right). \quad (123)$$

Additionally, in order to assess the accuracy of the Molière theory in determining the screening angle χ'_a , we also define the absolute and relative differences between the values of $\delta_M^{(2)}(\chi'_a)$ and $\delta_{CC}^{(2)}(\chi'_a)$ as well as between the $\delta_M^{(2)}(\chi'_a)$ and $\delta_{CC}(\chi'_a)$ by the relations

$$\delta_{CCM}^{(2)}(\chi'_a) = \frac{\Delta_{CCM}^{(2)}(\chi'_a)}{\delta_M^{(2)}} = \frac{\delta_M^{(2)} - \delta_{CC}^{(2)}}{\delta_M^{(2)}} = 1 - \frac{\delta_{CC}^{(2)}}{\delta_M^{(2)}}, \quad (124)$$

$$\delta_{CCM}(\chi'_a) = \frac{\Delta_{CCM}(\chi'_a)}{\delta_M^{(2)}} = \frac{\delta_M^{(2)} - \delta_{CC}}{\delta_M^{(2)}} = 1 - \frac{\delta_{CC}}{\delta_M^{(2)}}. \quad (125)$$

The numerical estimation of the second-order corrections shows that the values of the relative corrections $\delta_{CC}^{(2)}$ for heavy target atoms with $Z \sim 80$ does reach 40%. From it is also obvious that with the rise in the nuclear charge the absolute inaccuracy $\Delta_{CCM}^{(2)}(\chi'_a)$ of the Molière's theory in determining the screening angle χ'_a increases to approximately 16%, and the corresponding relative error $\delta_{CCM}^{(2)}(\chi'_a)$ does not depend on Z and is about 28%.

To estimate the exact ('Coulomb') corrections according to the formulas (113) and (117), we must first calculate the values of the function $f(a) = \Re[\psi(1+ia)] + C_E$.

From the digamma series [29]

$$\psi(1+a) = 1 - C_E - \frac{1}{1+a} + \sum_{n=2}^{\infty} (-1)^n [\zeta(n-1)] a^{n-1}, \quad |a| < 1, \quad (126)$$

where ζ is the Riemann zeta function, leads the corresponding power series for $\Re[\psi(1+ia)] = \Re[\psi(ia)]$

$$\Re[\psi(ia)] = 1 - C_E - \frac{1}{1+a^2} + \sum_{n=1}^{\infty} (-1)^{n+1} [\zeta(2n+1)] a^{2n}, \quad |a| < 2, \quad (127)$$

and the function $f(a) = a^2 \sum_{n=1}^{\infty} [n(n^2+a^2)]^{-1}$ can be represented as follows:

$$\begin{aligned} f(a) &= 1 - \frac{1}{1+a^2} + \sum_{n=1}^{\infty} (-1)^{n+1} [\zeta(2n+1)] a^{2n}, \quad |a| < 2, \quad (128) \\ &= 1 - \frac{1}{1+a^2} + 0.2021 a^2 - 0.0369 a^4 + 0.0083 a^6 - \dots \end{aligned} \quad (129)$$

The calculation results for Z dependence of (128), the relative CC and their difference with the Molière corrections, as well as the unitary corrections (97) at $\beta = 1$ are presented in Table 1.

Table 1. The Z dependence of the corrections defined by Eqs. (97), (113), (117), and (125)

M	Z	$Z\alpha$	$10 \delta_{unit}$	$f(Z\alpha)$	δ_{CC}	Δ_{CCM}	δ_{CCM}
Be	4	0.029	0.002	0.001	0.001	0.000	0.286
Al	13	0.094	0.007	0.011	0.011	0.004	0.280
Ti	22	0.160	0.012	0.031	0.031	0.012	0.280
Ni	28	0.204	0.015	0.049	0.050	0.020	0.287
Mo	42	0.307	0.022	0.105	0.110	0.047	0.297
Sn	50	0.365	0.027	0.144	0.154	0.068	0.306
Ta	73	0.533	0.039	0.276	0.318	0.157	0.330
Pt	78	0.569	0.041	0.307	0.359	0.182	0.336
Au	79	0.577	0.042	0.313	0.367	0.187	0.337
Pb	82	0.598	0.044	0.332	0.393	0.205	0.342

The Table 1 shows that while the values of relative unitary corrections δ_{unit} for heavy atoms of the target material does not reach 0.5%, the maximum value of the difference $\Delta_{CC} [\ln(\chi'_a)] = f(Z\alpha)$ is close to 33%, and the magnitude of the corresponding relative Coulomb correction δ_{CC} is reached for $Z \sim 80$ the value of order of 40%.

From it is also obvious that the absolute inaccuracy Δ_{CCM} of the Moliere's theory in determining the screening angle χ'_a with the rise of Z increases to 20% and the corresponding relative inaccuracy δ_{CCM} is about 34 percent. Thus, in the case of scattering on targets with large Z the such corrections as $\Delta_{CCM}(\chi'_a)$ and δ_{CCM} become significant and should be taken into account in determining the lifetimes of relativistic elementary atoms in experiments with nuclear targets.

4 Conclusion

1. Within the framework of unitary Glauber approximation for particle-atom scattering, we develop the general formalism of the Molière–Fano multiple scattering theory.
2. We have estimated the relative unitary corrections to the parameters of the M–F theory, resulting from a reconstruction of it's unitarity in second-order optical-model of the Glauber theory and found that they are of order $Z\alpha^2$.
3. We have also received the rigorous relations for the exact and the Born values of the quantities $Q_{el}(\eta)$, $\ln[g(\eta)]$, and χ'_a , which do not depend on the shape of the electron density distribution in the atom and are valid for any atomic model.
4. We have calculated the Coulomb corrections $\Delta_{CC} \equiv \Delta_{CC} [\ln(\chi'_a)] = \Delta_{CC} [\ln g(\chi_c)]$ and relative corrections $\delta_{CC} \equiv \delta_{CC}(\chi'_a) = \delta_{CC} [g(\chi_c)] = \delta_{CC} [W_M(\chi_c, t)]$ with nuclear charge ranged from $Z = 2$ to $Z = 82$ and showed that for $Z \sim 80$ these corrections comprise the order of 30% and 40%, correspondingly.
5. Additionally, we evaluated the absolute and relative inaccuracies of the Moliere's theory in determining the screening angle and found that for heavy atoms of the target material ($Z \sim 80$) they are about 20% and 30%, respectively.

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